

Simulation of Graphene Nanoribbon Field Effect Transistors

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Abstract

We present an atomistic three-dimensional simulation of graphene nanoribbon field effect transistors (GNR-FETs), based on the self-consistent solution of the 3D Poisson and Schrödinger equation with open boundary conditions within the non-equilibrium Green's Function formalism and a tight-binding Hamiltonian. With respect to carbon nanotube FETs, GNR-FETs exhibit comparable performance, reduced sensitivity on the variability of channel chirality, and similar leakage problems due to band-to-band tunneling. Acceptable transistor performance requires prohibitive effective nanoribbon width of 1-2 nm and atomistic precision, that could in principle be obtained with periodic etch patterns or stress patterns.

Keywords: graphene, nanoribbon, NEGF, three-dimensional Poisson, Atomistic tight-binding Hamiltonian.

I. INTRODUCTION

In the last decade, Carbon NanoTubes (CNT) have attracted extraordinary interest for their extremely interesting physical and electrical properties [1], and their potential as an alternative to silicon as channel material for transistors beyond CMOS technology [2]. Recent experiments by Novoselov et al. [3] demonstrated the possibility of fabricating stable single atomic layer graphene sheets, with remarkable electrical properties, that have brought new excitation to the field of carbon electronics.

Two-dimensional graphene is a zero gap material, which makes it not suitable for transistor applications.

Energy gap can however be induced by means of lateral confinement [4], realized for example by lithography definition of narrow graphene stripes, the so-called graphene nanoribbons.

Experiments on graphene-based devices [5] and Graphene NanoRibbon FETs [6] (GNR-FETs) have appeared only very recently, and demonstrate limited capability to modulate the conductance of a graphene channel at room temperature. The main problem is the need to fabricate extremely narrow nanowires (of the order of 1 nm) with atomic precision to obtain an energy gap adequate for room temperature operation.

Since at the moment the fabrication technology is at its very first steps, computer simulations can be very useful to provide physical insights of GNR-FETs and to estimate the attainable performance. Recent theoretical works have shown that graphene nanoribbons have an energy gap which has an oscillating behavior as a function of width, with average roughly proportional to the inverse width, and that edge states play a very important role in inhibiting the existence of fully metallic nanoribbons [7]. Such behavior cannot be reproduced if one does not consider edge effects [8].

Also from the simulation point of view, research on GNR-FETs is at an embryonic stage: the only works available in the literature [9], [10] are based on a semiclassical analytical top-of-the-barrier model. For short-channel transistors only a three-dimensional simulation is suitable for an accurate evaluation of the electrostatics and of intraband and interband tunneling.

To this purpose, we have developed a code for the simulation of GNR-FETs, based on the Non-Equilibrium Green's Function formalism (NEGF), with a tight-binding Hamiltonian built from p_z orbital basis set in the real space, which has been included in our in-house three-dimensional device simulator NANOTCAD ViDES [11]. We will show that GNR-FETs have performance comparable with CNT-FETs, and that can be greatly affected by the channel width and edge roughness.

II. PHYSICAL MODEL AND RESULTS

Our approach is based on the self-consistent solution of the three-dimensional Poisson and Schrödinger equations with open boundary conditions [12], which is able to take into account fully ballistic transport, in order to outline the higher limits of device performance, as well as elastic scattering due to line edge roughness. The Hamiltonian is taken from [7], in which edge states at the nanoribbon lateral ends have been considered. In this work we refer to $(N,0)$ armchair graphene nanoribbons, which consist of an unrolled $(n,0)$ zig-zag nanotube with $N = 2n$.

The considered double-gate GNR-FETs have the structure depicted in the inset of Fig. 1. The gates are metallic, the oxide thickness t_{ox} is equal to 1 nm, the channel is 15 nm long, and W is the channel width. The source and drain extensions are 10 nm long, and are doped with a molar fraction of fully ionized donors $f = 5 \times 10^{-3}$. The spacing between parallel GNRs is 4 nm.

In Fig. 1 the transfer characteristics of a (12,0) GNR-FET ($W=1.37$ nm) for drain-to-source voltage V_{DS} of 0.1 and 0.5 V are shown, and compared to those of a (16,0) CNT-FET with the same geometry (same t_{ox} , L and device spacing), whose energy gap (E_{gap}) is close to that of the GNR-FET and equal to 0.6 eV.

Good control of the channel by the gate potential is shown at $V_{DS}= 0.1$ V, since the sub-threshold swing (S) for the GNR-FET and the CNT-FET are 64 and 68 mV/dec, respectively. For $V_{DS}= 0.5$ V we observe a pronounced degradation of S , with $S=191$ mV/dec for the GNR-FET and almost 250 mV/dec for the CNT-FET. This has to be imputed to Hole-Induced Barrier Lowering (HIBL) [12] : in the sub-threshold regime, when sufficiently high V_{DS} is applied, confined states in the valence band of the channel align with the occupied states in the drain, leading to band-to-band injection of holes in the channel.

If only elastic band-to-band tunneling can occur (as assumed in our simulation) the excess of holes in the channel lowers the channel potential, increasing the off current and S , as shown in Fig. 1: the lower the energy gap and the higher the V_{DS} , the higher the HIBL effect. HIBL is more pronounced in CNT-FETs than in GNR-FETs, because the conduction band of CNTs is double degenerate and therefore CNTs have twice the density of states of GNRs with the same gap.

If, on the other hand, inelastic band-to-band tunneling or Shockley-Read-Hall mechanisms are relevant, holes can recombine with electrons at the source and, instead of HIBL, we observe a leakage current from source to drain due to gate-induced drain leakage (GIDL) [13].

In strong inversion, the transconductance g_m at $V_{DS}=0.1$ V is 3600 and 6100 $\mu\text{S}/\mu\text{m}$ for the GNR-FET and the CNT-FET, respectively, whereas at $V_{DS}=0.5$ V, we obtain $g_m=4800 \mu\text{S}/\mu\text{m}$ for the GNR and a $g_m=8760 \mu\text{S}/\mu\text{m}$ for the CNT. The advantage of CNT-FETs is due to the double degeneracy of the conduction band in carbon nanotubes.

It is known that a variability of the chirality of fabricated CNTs yields metallic nanotubes useless for transistor applications. For GNRs this problem is mitigated, since all GNRs are semiconducting. In order to investigate quantitatively the effect of a finite fabrication tolerance on the width of GNRs, we have computed the transfer characteristics of GNR-FETs with different chiralities : (12,0), (14,0) and (16,0).

As can be seen in Fig. 2a, the three devices behave as transistors, but show very different behavior, even if they differ by only one carbon atom along the channel width. The problem is that the gap is still largely dependent on the chirality : the (16,0) GNR ($W=1.87$ nm) has the larger gap ($E_{gap} = 0.71$ eV), while the (14,0) ($W=1.62$ nm) has the smallest gap ($E_{gap} = 0.13$ eV). As a consequence, the (16,0) device show the best gate control over the channel potential, while the (14,0) the worst : the energy gap is so small that elastic band-to-band tunneling occurs at the source and current is dominated by GIDL.

Such problem is reduced if rough edges are considered. We have considered the impact of line edge roughness in a (16,0) GNR-FET device, by randomly decoupling carbon atoms on the lateral boundaries of the GNR. The transfer

characteristic for one example is shown in Fig. 2 (dashed line). Since the channel consists of several hundreds of rings, the rough GNR behaves as a GNR with an intermediate effective gap. More statistical simulations would be needed to assess the dispersion of the electrical characteristics, but the typical GNRs is probably long enough to provide sufficient averaging to suppress inter device dispersion. Rough edge scattering strongly affects the on-current and the transconductance suppressing it by about 30% with respect to fully ballistic transistors. Additional suppression in realistic GNR-FETs can be due to defects, ionized impurities and phonon scattering.

From the above simulations, it is clear that lateral confinement way beyond state-of-the-art etching capabilities would be needed to obtain adequate E_{gap} . We also found that electrostatic periodic potential modulation with a peak-to-peak value of few Volts is not sufficient to induce the required gap of few hundreds mV.

In order to evaluate whether a periodic strain pattern can allow to engineer the GNR gap, we have computed the energy gap in a (24,0) GNR ($W=5.86$ nm), multiplying the overlap integral of the element of the Hamiltonian in correspondence of the couple of atoms in the middle of the GNR by a "strain factor" σ : σ is larger than one for compressive strain, and smaller than one for tensile strain. As can be seen in Fig. 3, compressive strain seems to be able to increase the energy gap of the nanowire by a significant amount. Of course, we can only suggest to experimentalists to evaluate the option.

III. CONCLUSIONS

In this work, a simulation study of GNR-FETs has been performed by means of the self-consistent solution of the 3D Poisson and Schrödinger equation with open boundary conditions, within the NEGF formalism. Edge states have been considered at the lateral ends of the nanoribbon using the model proposed by [7]. GNR-FETs exhibit performance similar to CNT-FETs, also showing significant band-to-band tunneling when small gap devices are considered and large V_{DS} is applied. GNR-FETs are more robust than CNT-FETs with respect to variability of the channel chirality, and edge roughness seems to play an useful averaging effect. Finally we suggest that periodic strain could in principle represent an alternative to etching for inducing an energy gap in graphene.

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Fig. 1. Transfer characteristics of double-gate CNT and GNR-FETs, with doped source and drain reservoirs, with channel length equal to 15 nm, oxide thickness t_{ox} equal to 1 nm and channel width $W=1.37$ nm. The lateral space is equal to 2 nm. In the inset, a sketch of the GNR-FET is shown.

Fig. 2. Transfer characteristics in the logarithmic a) and linear b) scale of GNR-FETs with different chiralities (12,0), (14,0) and (16,0) (channel width W equal to 1.37 nm, 1.62 nm and 1.87 nm, respectively), for $V_{DS}=0.1$ V. The transfer characteristic for the (16,0) GNR-FET, when roughness at the lateral edge of the GNR is considered is also shown (dashed line). In the inset, a sketch of the graphene nanoribbon is shown, where randomly decoupled atoms have been highlighted (thick lines).

Fig. 3. Energy gap of a (24,0) GNR, when tensile and compressive strain is considered in correspondence of the middle of the nanoribbon, as a function of the strain factor by which the Hamiltonians elements of the strained carbon atoms are multiplied.

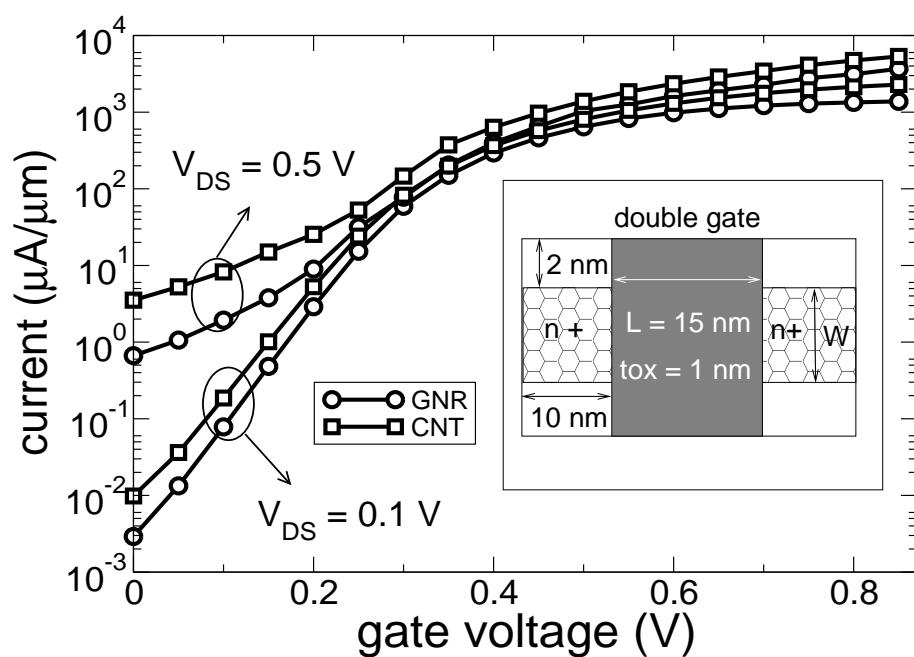


FIG. 1

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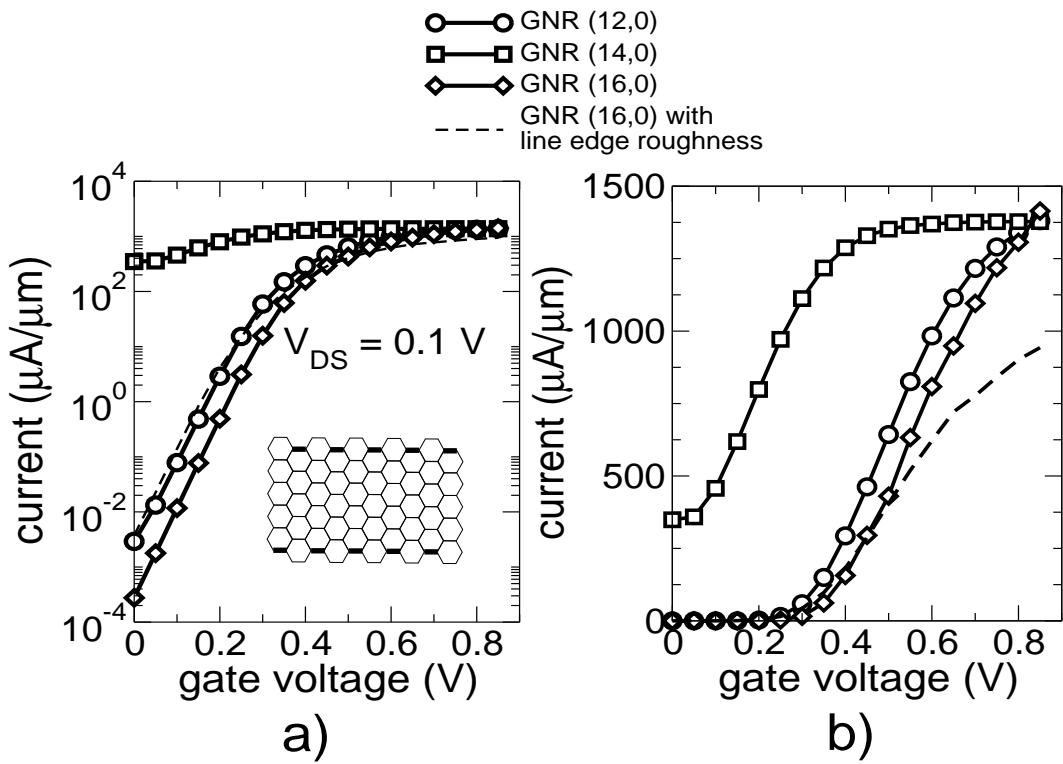


FIG. 2

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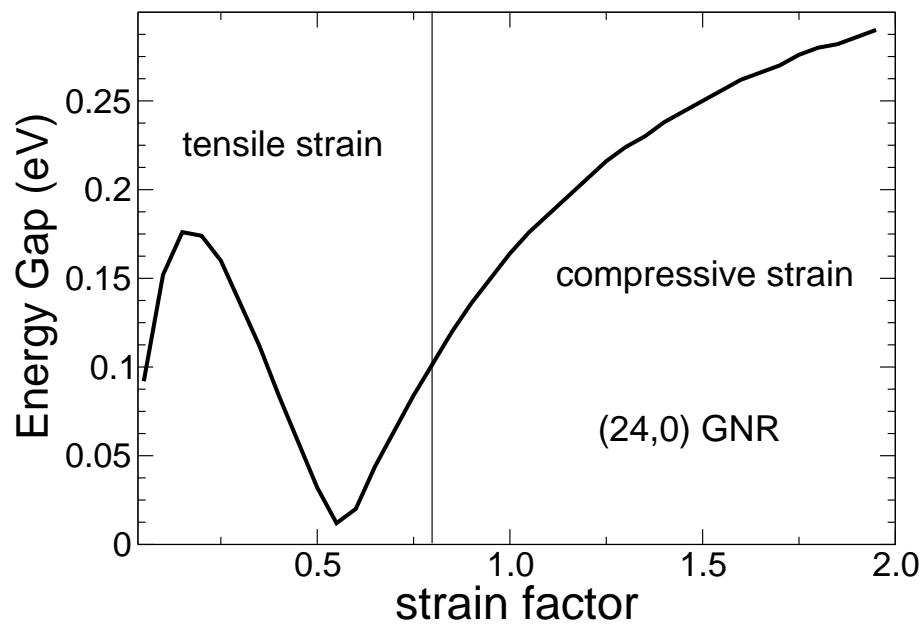


FIG. 3

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